On the Coulomb Sturmian matrix elements of relativistic Coulomb Green's operators

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Abstract

The Hamiltonian of the radial Coulomb Klein-Gordon and second order Dirac equations are shown to possess an infinite symmetric tridiagonal matrix structure on the relativistic Coulomb Sturmian basis. This allows us to give an analytic representation for the corresponding Coulomb Green's operators in terms of continued fractions. The poles of the Green's matrix reproduce the exact relativistic hydrogen spectrum.

I. INTRODUCTION

In quantum mechanics the knowledge of the Green's operator is equivalent to the complete knowledge of the system. So, having an analytic basis representation for the Green's operator can tremendously simplify the actual calculations. If we know the Green's operator only of the asymptotic part of the Hamiltonian we can treat the remaining terms as perturbations and approximate them by finite matrices.

In a recent publication, Ref. [1], we have proposed a method for calculating matrix representation of Green's operators. If, in some basis representation, the Hamiltonian possesses an infinite symmetric tridiagonal (Jacobi) matrix structure the corresponding Green's operator can be given in terms of continued fractions. In Ref. [1], this theorem were exemplified with the Green's operator of the non-relativistic Coulomb and harmonic oscillator Hamiltonian, and, in Ref. [2], an exactly solvable non-relativistic potential problem were considered which provides a smooth transition between the Coulomb and the harmonic oscillator problems.

The aim of this paper is to extend this result for relativistic Coulomb Green's operators, i.e., for the Coulomb Green's operator of the Klein-Gordon and of the second order Dirac equations. This later is equivalent to the conventional Dirac equation and seems to have several advantages. For details see Ref. [3] and references therein. The Coulomb Sturmian matrix elements of the second order Dirac equation has already been obtained by Hostler [3] via evaluating complicated contour integrals. Our derivation, however, is much simpler, it relies only on the Jacobi-matrix structure of the Hamiltonian, and the result obtained

is also better suited for numerical calculations. In Ref. [3] the result appears in terms of Γ and hypergeometric functions, while our procedure results in an easily computable and analytically continuable continued fraction.

II. MATRIX ELEMENTS OF RELATIVISTIC COULOMB–GREEN'S OPERATORS

The radial Klein-Gordon and second order Dirac equations for Coulomb interaction are given by

$$H_u \left| \xi^u \right\rangle = 0, \tag{1}$$

where

$$H_u = \left(\frac{E}{\hbar c} \right)^2 - \mu^2 + \frac{2\alpha Z}{\hbar c} \frac{E}{r} + \frac{d^2}{dr^2} - \frac{u\,(u+1)}{r^2}. \tag{2}$$

Here $\mu = mc/\hbar$, $\alpha = e^2/\hbar c$, m is the mass and Z denotes the charge. For the Klein-Gordon case u is given by

$$u = -\frac{1}{2} + \sqrt{\frac{1}{4} + l(l+1) - (Z\alpha)^2}, \tag{3}$$

and in the case of the second order Dirac equation for the different spin states we have

$$u_\pm = -\frac{1}{2} \mp \frac{1}{2} + \sqrt{\left(j + \frac{1}{2} \right)^2 - (Z\alpha)^2}. \tag{4}$$

The relativistic Coulomb Green's operator is defined as the inverse of the Hamiltonian H_u:

$$H_u G_u = G_u H_u = \mathbf{1}_u, \tag{5}$$

where $\mathbf{1}_u$ denote the unit operator of the radial Hilbert space $\mathcal{H}_u$.

In complete analogy with the non-relativistic case we can define the relativistic Coulomb Sturmian functions as solutions of the Sturm-Liouville problem

$$\left(-\frac{d^2}{dr^2} + \eta^2 + \frac{u\,(u+1)}{r^2} - \frac{2\eta(n+u+1)}{r} \right) S_{n;\eta}^u(r) = 0, \tag{6}$$

where η is a real parameter and $n = 0, 1, 2, \ldots, \infty$ is the radial quantum number. In coordinate space representation they take the form,

$$\left\langle r \left| nu; \eta \right\rangle = \left[\frac{n!}{(n+2u+1)!} \right]^{\frac{1}{2}} (2\eta r)^{u+1} e^{-\eta r} L_n^{2u+1}(2\eta r), \tag{7}$$

where L is a Laguerre-polinom. The Coulomb Sturmian functions, together with their biorthogonal partner $\left\langle r \left| \widetilde{nu; \eta} \right\rangle = 1/r \cdot \left\langle r \left| nu; \eta \right\rangle \right.$, form a basis: i.e., they are orthogonal,

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$$\langle \widetilde{nu; \eta} \, | mu; \eta \rangle = \langle nu; \eta \, | \widetilde{mu; \eta} \rangle = \delta_{nm}, \tag{8}$$

and form a complete set in $\mathcal{H}_u$

$$\sum_{n=0}^{\infty} |nu; \eta\rangle\langle \widetilde{nu; \eta}| = \sum_{n=0}^{\infty} |\widetilde{nu; \eta}\rangle \langle nu; \eta| = \mathbf{1}_u. \tag{9}$$

A straightforward calculation yields:

$$\langle nu; \eta | mu; \eta \rangle = \frac{1}{2\eta} \Big[\delta_{nm}(2u + 2n + 2) - \delta_{nm-1}\sqrt{(n+1)(n+2u+2)}$$
$$- \delta_{nm+1}\sqrt{n\,(2u+n+1)} \Big]. \tag{10}$$

Utilizing this relation and considering Eq. (6) we can easily calculate the Coulomb Sturmian matrix elements of H_u,

$$\underline{H}_{nm} := \langle nu; \eta | \, H_u \, | mu; \eta \rangle =$$

$$+ \delta_{nm} \left(\frac{2\alpha z E}{\hbar c} - 2(u+n+1)\eta + 2(u+n+1)\frac{(E/\hbar c)^2 - \mu^2 + \eta^2}{2\eta} \right)$$

$$- \delta_{nm-1} \left(\frac{(E/\hbar c)^2 - \mu^2 + \eta^2}{2\eta} \sqrt{(n+1)(n+2u+2)} \right) \tag{11}$$

$$- \delta_{nm+1} \left(\frac{(E/\hbar c)^2 - \mu^2 + \eta^2}{2\eta} \sqrt{n(n+2u+1)} \right),$$

which happens to possess a Jacobi-matrix structure. So, the theorem of Ref. [1] is readily applicable here.

Let us consider the $\infty \times \infty$ Green's matrix

$$(\underline{G}_u)_{nm} \equiv \langle \widetilde{nu; \eta} | G_u | \widetilde{mu; \eta} \rangle, \tag{12}$$

and let us denote its rank-N leading principal submatrix by $\underline{G}_u^{(N)}$. Then, according to Ref. [1],

$$(\underline{G}_u^{(N)})_{ij}^{-1} = \underline{H}_{ij} + \delta_{jN} \, \delta_{iN} \, \underline{H}_{iN+1} \, \mathcal{F}, \tag{13}$$

where $\mathcal{F}$ is a continued fraction

$$\mathcal{F} = -K_{i=N}^{\infty} \left(\frac{a_i}{b_i} \right) = -\frac{a_{1+N}}{b_{1+N}} + \frac{a_{2+N}}{b_{2+N}} + \cdots + \frac{a_{n+N}}{b_{n+N}} + \cdots, \tag{14}$$

whose coefficients are related to the Jacobi matrix

$$a_i = -\frac{\underline{H}_{ii-1}}{\underline{H}_{ii+1}}, \quad b_i = -\frac{\underline{H}_{ii}}{\underline{H}_{ii+1}}. \tag{15}$$

This continued fraction convergent for bound-state energies, but, by using the method presented in Ref. [1], can be continued analytically to the whole complex energy plane. Simple matrix inversion gives now the desired Green's matrix.

In Table I we demonstrate the numerical accuracy of method by evaluating the ground and some highly excited sates of relativistic hydrogen-like atoms, which, in fact, correspond to the poles of the Dirac Coulomb Green's matrix. In particular, the zeros of the determinant of (13) were located. It should be noted that irrespective of the rank N the zeros should provide the exact Dirac results. In Table I we have taken 2×2 matrices. Indeed, the results of this method, E_{cf}, agree with the exact one in all cases, practically up to the machine accuracy, allowing thus to study the fine structure splitting.

III. SUMMARY

In this short note we have presented a practical and easy-to-apply procedure for calculating the Coulomb Sturmian matrix elements of the Coulomb Green's operator of the Klein-Gordon and of the second order Dirac equations. The method is relied only on the Jacobi-matrix structure of the corresponding Hamiltonians and results in a continued fraction which can be continued analytically to the whole complex energy plane.

ACKNOWLEDGMENTS

TABLES

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	energy levels	E_{cf}	E_{D}	E_{S}
hydrogen $Z = 1$	$1\text{S}_{1/2}$	-0.5000066521	-0.5000066521	-0.5
	$2\text{P}_{1/2}$	-0.1250020801	-0.1250020801	-0.125
	$2\text{P}_{3/2}$	-0.1250004160	-0.1250004160	-0.125
	$50\text{P}_{1/2}$	-0.0002000002	-0.0002000002	-0.0002
	$50\text{P}_{3/2}$	-0.0002000001	-0.0002000001	-0.0002
uranium	$1\text{S}_{1/2}$	-4861.1483347	-4861.1483347	-4232
	$100\text{D}_{3/2}$	-0.4241695002	-0.4241695002	-0.4232
	$100\text{D}_{5/2}$	-0.4238303306	-0.4238303306	-0.4232

TABLE I. Energy levels of hydrogen-like atoms in atomic units. E_{cf} is the relativistic spectrum calculated via continued fraction, E_{D} and E_{S} are textbook values of the relativistic Dirac and the non-relativistic Schrödinger spectrum, respectively.

REFERENCES

[1] B. Kónya, G. Lévai and Z. Papp, J. Math. Phys., **38**, 4832 (1997).

[2] G. Lévai, B. Kónya and Z. Papp, J. Math. Phys., **39**, 5811 (1998).

[3] L. C. Hostler, J. Math. Phys. **28**, 2984 (1987).